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The M-G Hamiltonian - a pedagogic review

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Abstract : In this review, we discuss Majumdar-Ghosh Hamiltonian which is a one dimensional system of spin 1/2 particles with isotropic interactions between nearest and next-nearest neighbours. The model is exactly solvable when the next-nearest neighbour strength is half that between the nearest neighbours. The ground state is doubly degenerate and consists of dimers of nearest neighbour singlet pairs.

Keywords · Majumdar-Ghosh chain, Heisenberg model, Haldane conjecture, Haldane-Shastry model

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1. Introduction

Heisenberg model of spin-spin interaction has been a work horse for researchers in studying magnetic properties of materials. From a phenomenological point of view, Heisenberg model is a simple bilinear coupling of spins at adjacent sites in a crystal through a rotationally invariant interaction. Heisenberg type spin spin interaction could arise by direct exchange interaction or indirectly from a process known as *superexchange*. Effective interaction of this form could also be applicable to itinerant spin systems through an indirect interaction.

For simplicity, we consider atoms with orbitally non-degenerate ground states, *i.e.* with $L = 0$, so that the total angular momentum J is the same as the spin angular momentum S. We assume that such atoms are separated by sufficiently large distances so that the interaction between them is weak. In the Heisenberg model the electronic degrees of freedom are neglected and only the spin degree of freedom plays a dominant role. Magnetism arises from a collective behaviour of electrons in the valence shell of these atoms, which have stable microscopic magnetic moments at low temperatures. In a ferromagnetic solid this collective behaviour results in a tendency of the magnetic moments at the nearest neighbour sites to be aligned parallel, giving a configuration of the type $|\uparrow\uparrow\uparrow...\uparrow\rangle$. In an antiferromagnet the nearest neighbour spins are aligned anti-parallel. In the Heisenberg model, the interaction between two adjacent spins is in the nature of scalar product of spin operators at the sites. If the sites are labelled l and m, the interaction is of the form $J\ \boldsymbol{S}_l \cdot \boldsymbol{S}_m$, where J is a constant called the exchange constant.

The Heisenberg model of spin-spin interaction is therefore written in the following form

$$H = J\sum \boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{1}$$

The M-G Hamiltonian[1], proposed by Majumdar and the present author is essentially a one dimensional Heisenberg model with both the nearest and next-nearest neighbour exchange interaction. The model is exactly solvable for a particular ratio of these two exchange constants and has a two-fold degenerate dimer ground state with arose from a study of Heisenberg model in one dimension, further comments are confined to one dimension.

2. Heisenberg ferromagnet

It is convenient to rewrite the model Hamiltonian in terms of spin raising a lowering operators S^+ and S^- by

$$S^{\pm} = S^x \pm iS^y \cdot$$

These operators satisfy the following commutaion rules

$$\left[S_i^+, S_j^-\right] = 2\delta_{i,j}S_i^z,$$

$$\left[S_i^z, S_j^{\pm}\right] = \pm S_i^{\pm},$$

where $\delta_{i,j} = 0$ for $i = j$ and is zero otherwise. S_i^+ has the property that it increases the z component of the spin at the i-th site by one. Likewise S_i^- decreases the value of S_i^z by one. For $S = 1/2$, because of the impossibility of having more than one spin deviation at a site, we have the constraint

$$(S^{\pm})^2 = 0 .$$

For a general value of spin, this constraint becomes $(S^{\pm})^{2S+1} = 0$. In terms of these operators, the Hamiltonian is expressed as

$$H = 2J \sum \left| \frac{S_i^- S_{i+1}^- + S_i^+ S_{i+1}^+}{2} + S_i^z S_{i+1}^z \right| .$$

Instead of considering an open chain, we consider a ring configuration, so that the $(N + 1)$-th spin is a neighbour of the N-th spin.

Using the above form of the Hamiltonian, it is easy to see that the ground state energy of the ferromagnetic state in which all spins are aligned is given by $JN/2$. For a general spin S, the ground state is one in which the value of S^z at individual sites take the maximum value S and the ground state energy is $2JNS^2$.

As the temperature is increased from zero, some of the individual spins deviate from their ground state value. For a general value of spin S, the lowest excitation corresponds to the case where the value of S^z at one of the sites deviates from its maximum value $+S$ to a value $S - 1$, or equivalently, from $-S$ to $S + 1$. For the case of spin one-half, taking the ground state to be one in which all spins are down, a possible excited state is one in which one of the sites has a spin up. However, because of the fact that the spins in the adjacent sites are coupled by exchange interaction, the deviated state does not remain confined to a particular site but moves from site to site as a wave like disturbance. The energy of the excited state can be shown to be equal to $E_k = J(1 \cos ka)$ with respect to the ground state, where k is the wave number asscociated with the excitation. Such excitations are known as *spin waves*.

Pictorially, it is easy to visualize spin wave by regarding spin as a classical vector so that spins precess with a phase shift about the direction in which they point in the ground state (Figure 1). Note that the spectrum of energy is gapless in the sense that in the long wavelength limit $(k \to 0)$, $E_k = Dk^2$,

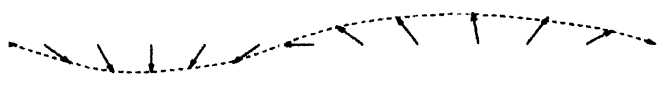

Figure 1. Spin wave excitation in a classical ferromagnet. The spin vector precesses about the z-axis.

which is continuous with the ground state energy. D is called the stiffness constant of the spin wave. Quantized spin waves are known as magnons.

Interest in the higher excited states consisting of bound states of two reversed spins arose due to observation of bound state complexes of excitations in one dimensional magnon systems. Two spin deviate state, which in case of spin half corresponds to reversal of spins at two sites in the crystal, could just be two independent spin waves propagating in the crystal. Alternatively, it could be a situation in which these two sites are adjacent to each other and the disturbance moves in a coherent fashion as a bound state. Theoretically, the existence of bound states in the Heisenberg system was established by pioneering work of Wortis[2]. Majumdar [3] investigated the dependence of these bound states on the strength of the next nearest neighbour interaction and found that these bound states merge into continuum as the strength of the next nearest neighbour interaction increases. Majumdar and co-workers [4-6] also looked into the problem of deviation of three spins from the ground state ,using a technique due to Faddeev . They used the Dyson Hamiltonian of ideal bosonic spin waves instead of considering the spin operators themselves. The disadvantage of this Hamiltonian is that it does not reproduce the kinematical constraint of the impossibility of reversing two spins at the same site and leads to additional bound states, in addition to the real ones. However, they were able to identify these unphysical bound states by a simple prescription and obtain simple Faddeev equations.

3. Ground state and excitations of an antiferromagnetic chain

In contrast to the case of ferromagnet, the antiferromagnetic case presents enormous difficulties. If one regards spin as a classical vector, the lowest energy state would be one in which the spin at a particular site is surrounded by spins which point in the opposite direction.This is known as the Néel state Unfortunately, the classical Néel state is not even an eigen state of the Heisenberg Hamiltonian. Evèn the one dimensional antiferromagnetic chain poses enough mathematical diffculties For $S = 1/2$ Hulthén [7] had obtained the ground state energy using an algebraic technique called the *Bethe Ansatz* [8]. The ground state is a linear combination of ${}^{N}C_{N/2}$ states having $N/2$ spins pointing down and an equal number pointing up. The energy of the ground state is given by

$$E_0 = \frac{1}{2} N J (4 \ln 2 - 1) = -0.443 JN . \qquad (2)$$

The spectrum of excitation of one dimensional antiferromagnetic chain was obtained by des Cloizeaux and Pearson [9] , who found that magnon excitations are gapless, *i.e.*, there exists excitations with arbitrarily low energy

immediately above the ground state energy. These excitations are given by

$$\omega_k = J|\sin k|. \tag{3}$$

There are actually two degenerate antiferromagnetic spin wave modes whose frequencies vanish at $k \to 0$ and $k \to \pi$. However, these excitations are different from the spin waves of the type considered for ferromagnets in that these are not small fluctuations about a ground state with broken symmetry. Figure 2 shows the excitation spectrum of a one dimensional antiferromagnetic chain.

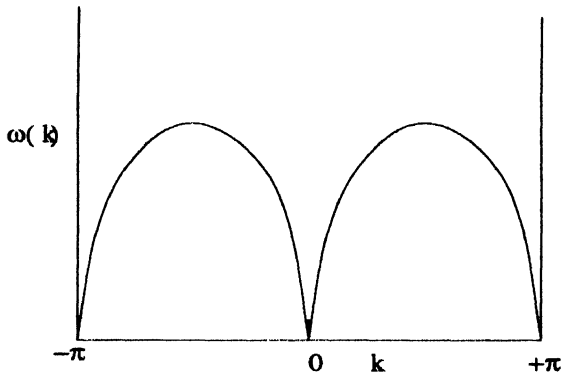

Figure 2. Antiferromagnetic spin waves.

The correlation between a pair of spins decreases with distance following a power law behaviour. As the temperature is raised above $T = 0$, one expects that these correlations would be reduced further and ultimately disappear above some critical temperature T_c. However, an exact theorem due to Mermin and Wagner [10] shows that contrary to above expectation, there exists no magnetic ordering even for temperatures infinitisimally above absolute zero.

4. The Haldane conjecture and valence bond solid

We have seen that for both ferromagnetic and antiferromagnetic case, the low lying excitations are such that in the long wavelength limit, the excitation spectrum merges with the ground state with no gap. In 1983, Haldane [11] made a fascinating conjecture that Heisenberg chain with integral spins has a disordered ground state, above which, a finite excitation gap opens up, while the half odd integral spin chains have a critical ground state and a gapless excitation. The prediction has since been verified both numerically and experimentally. This *gapped* Haldane phase for integral spin systems is characterized by a spin correlation function which decays exponentially with distance.

$S = 1$ spin chain can be understood in terms of valence bond solid (VBS) solid model. A valence bond is formed from two spin 1/2's at two adjacent (or distant) sites in a lattice coupled to a singlet $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$. $S = 1$ spin on each site is represented as a symmetrized product of two spin 1/2 's at the same site. One can form a valence bond solid out of these by first forming a valence bond of two spin 1/2's at two adjacent sites and then symmetrizing the spins at the same site to restore the original $S = 1$ at the site. It has been shown rigorously that the correlation function decays exponentially in the valence bond state and there exists an energy gap.

Before discussing valence bond solids, we discuss the precursor to all such Hamiltonians, Majumdar and the present author had proposed in 1969 [1]. We performed numerical calculation on finite spin chains. Believing the ground state to be product of singlet states between adjacent pairs, we considered a basis consisting of such singlet products. In view of the limitations of computation imposed by the then existing CDC 3600 computer at TIFR, our numerical effort was limited to considering chains containing 4, 6, 8 and 10 spins ($S = 1/2$) on a ring. For $N = 10$, the number of states in the space $S^z = 0$ is ${}^{10}C_5 = 252$ and that with $S^z = 1$ is ${}^{10}C_4 = 210$. Recalling that both $S = 0$ and higher values of total spin S has projection in both $S^z = 0$ and $S^z = 1$ subspace while $S = 0$ does not have a projection in $S^z = 1$ subspace, the number of states which has spin zero is simply given by the difference between these two numbers. Thus, there are 42 states with the total spin $S = 0$. We worked with the following basis

$$\varphi_1 = [12][34][56][78][90],$$

$$\varphi_2 = [23][45][67][89][01], \tag{4}$$

where site 0 is written for 10 and

$$[lm] = \sqrt{\frac{1}{2}[\alpha(l)\beta(m) - \beta(l)\alpha(m)]}, \tag{5}$$

where α and β are the spin up and spin down states. The state $[l; m]$ represents a valence bond state between the adjacent sites l and m. The Hamiltonian we took was the next nearest neighbour Heisenberg Hamiltonian

$$H = 2J\sum_{i=1}^{N} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + 2J\alpha\sum_{i=1}^{N} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2} \tag{6}$$

with periodic condition $N+1 \equiv 1$ and $N+2 \equiv 2$. In the Hamiltonian, α is a parameter which denotes the strength of the next nearest neighbour interaction relative to the nearest neighbour interaction. A positive value of α indicates that the interaction between the nearest neighbours as well as that between the next neares neighbours are antiferromagnetic in nature. To our knowledge this is the first attempt in introducing *frustration* in a Heisenberg system. As the interaction between

nearest neighbours is antiferromagnetic, the interaction tends to align two such neighbours anti-parallel. To stabilize this configuration, it is necessary that the next nearest neighbour interaction has a ferromagnetic character as is the case with Nèel state. When the next nearest neighbour interaction has the same sign as that between the nearest neighbours, there is a competition between these two interactions. This is called frustration. Explicitly operating the Hamiltonian on the two functions given above resulted in a total of 40 more states. The resulting matrix was explicitly diagonalized. The result of numerical calculation is shown in Figure 3.

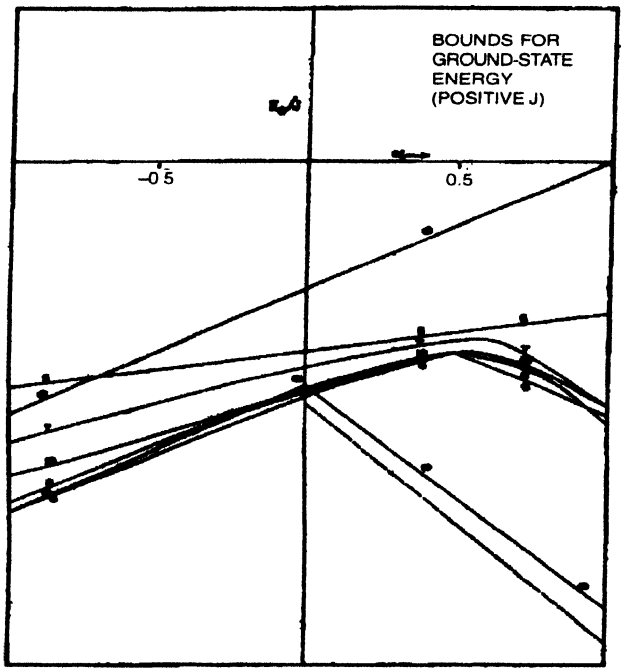

Figure 3. Ground-state energy per spin for $J > 0$. The curve marked ∞ are bounds obtained directly from Ref. [8]. The dashed curve is obtained by Majumdar and Ghosh [1].

The ground state energy curves for all even chains seemed to pass through an energy value

$$E_\infty / N = -0.75 .$$

This indicated existence of an exact answer. We considered two states defined by

$$\phi_1 = [12][34] \ldots [N-1; N],$$

$$\phi_2 = [23][45] \ldots [N, 1]. \qquad (7)$$

The basis functions of eq. (7) satisfy the following identity:

$$[k,l][m,n]+[k,n][l,m]+[k,m][n,l]=0. \qquad (8)$$

Using the properties of spin operators, one can show that

$$\left(\frac{1}{2}-2\boldsymbol{S}_l\cdot\boldsymbol{S}_m\right)[l,m]=2[l,m],$$

$$\frac{1}{2}-2\boldsymbol{S}_l\cdot\boldsymbol{S}_m\,\Big|[k,l][m,n]=[l,m][n,k].$$

By direct calculation, one can show that

$$H\phi_1 = -\frac{3}{2}NJ(1+\alpha)\phi_1 - J(1-2\alpha)\{[2,3][4,1]\ldots[N,N-1]$$

$$+[1,2][4,5]\ldots[N-1,N]+\ldots+[N,1][3,4]\ldots[2,N-1]\}$$

For $\alpha = 0.5$, $H\phi_1 = -(3/4)\,NJ\phi_1$, so that as $N \to \infty$, the energy per spin is $-3J/4$. Similarly, one can show that ϕ_2 is yet an eigenfunction of the Hamiltonian, degenerate with ϕ_1 are exact eigen states with the above energy. Pashupathy [12] showed that the variational estimate given by us is also a lower bound. This is shown by noting

$$J\sum_l(\boldsymbol{S}_l+\boldsymbol{S}_{l+1}+\boldsymbol{S}_{l+2})^2$$

$$=J\sum_l\left[S_l^2+S_{l+1}^2+S_{l+2}^2+2(\boldsymbol{S}_l\cdot\boldsymbol{S}_{l+1}+\boldsymbol{S}_{l+1}\cdot\boldsymbol{S}_{l+2}+\boldsymbol{S}_l\cdot\boldsymbol{S}_{l+2})\right]$$

As the triad of spins can give either $S = 1/2$ or $S = 3/2$, we have

$$\frac{1}{2}\left(\frac{1}{2}+1\right)J \le 3\frac{3}{4}J+2\langle H\rangle,$$

so that

$$\langle H\rangle \ge -\frac{3}{4}J .$$

The essential of the above proof lies in the realization that MG Hamiltonian,essentially projects out $S = 3/2$ state from a triad of adjacent spins. To see this let us rewrite the MG Hamiltonian [13] with a different strength parameter and add a constant term to the Hamiltonian. Let

$$H_{MG} = \frac{4J}{3}\sum_{i=1}^{N}\left(\boldsymbol{S}_i\cdot\boldsymbol{S}_{i+1}+\frac{1}{2}\boldsymbol{S}_i\cdot\boldsymbol{S}_{i+2}\right)+\frac{NJ}{2}. \qquad (9)$$

Considering a triad of spins at the sites i; $i+1$ and $i+2$, as shown above we have

$$\left(S_i^{tr}\right)^2 = (\boldsymbol{S}_{i-1}+\boldsymbol{S}_i+\boldsymbol{S}_{i+1})^2$$

$$=\frac{9}{4}+2\boldsymbol{S}_i\cdot(\boldsymbol{S}_{i+1}+\boldsymbol{S}_{i-1})+2\boldsymbol{S}_{i+1}\cdot\boldsymbol{S}_{i-1}.$$

Summing over i, one can easily see that

$$H_{MG} = \frac{1}{2} J \sum \left(S_i^{tr}\right)^2 - \frac{3}{2} N J$$

As $\left(S_i^{tr}\right)^2$ takes values 15/4 for $\left(S_i^{tr}\right)$ = 3/2 and 3/4 for $\left(S_i^{tr}\right)$ = 1/2, the eigenvalue of H_{MG} is zero in the singlet state. Since out of any triad a pair has $S^z = 0$, the third one can give only total $S^z = 1/2$. However, this cannot be a projection of $S = 3/2$ because we could then perform a rotation about a spin axis and add a component of $S^z = 3/2$ to the ground state, which is contrary to the rotational invariance of the Hamiltonian.

5. Resonating valence bond and MG hamiltonian

Valence bond states [14] are variational wave functions for antiferromagnetic models. They have been studied extensively in connection with quantum magnetism and superconductivity. In the context of Heisenberg model, the first such state to be proposed was the M-G Hamiltonian discussed above. These are situations where the spins are coupled in such a way that the entire system consists of clusters with $S = 0$. In cases where many such configurations are possible, the configurations have been called resonating valence bond (RVB). We have seen that ϕ_1 and ϕ_2 are degenerate ground states for the MG Hamiltonian. The state can be pictorially represented in terms of "dimers", which are singlet bonds between nearest neighbours only (Figure 4)

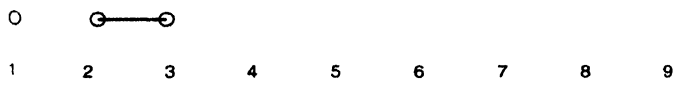

Figure 4. Dimer states in M-G chain

Shastry and Sutherland [15] have analyzed the excitation spectrum of MG chain. Established belief on excitations of quantum spin system was that the excitations are either spinons with spin one-half or are triplets having spin one. For instance, the one dimensional spin half Heisenberg model has only spinon excitation spectrum. However, with dimerization, the situation becomes complicated as some of the spinons get confined and the spectrum, therefore, consists of spinons and triplets. Shastry and Sutherland visualized the elementary excitation of MG chain to consist of two isolated non-interacting spinons in an otherwise dimerized nearest neighbour pairs.

Figure 5. Propagation of spinons in M-G chain

Figure 5 shows a pair of spinons on MG chain. The spinons are prevented from passing through each other because of dimerisation. With such a state as a variational wavefunction, one can show that the excitation energies are given by

$$\varepsilon_k = \frac{5J}{4} + J \cos 2k \,. \tag{10}$$

The minimum energy of excitation is therefore $J/4$. Affleck *et al* [16] have provided a rigorous proof of the existence of a gap in the MG model.

The ground state of MG chain has the following properties :

i. The translational symmetry is broken from a period 1 to a period 2 as can be seen from an examination of the structure of either of the two degenerate states.

ii. Excitation spectrum has a gap.

iii. Spin correlations are extremely short ranged. Even in the absence of next nearest neighbour interactions, there is no Néel order seen in the ground state and the spin correlations decay according some power law. The next nearest neighbour interaction frustrates the nearest neighbour interaction and further reduces correlations to one lattice distance.

The degenerate ground state of the model may be thought of as RVB state which restores the translational symmetry.

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